

10/522,622 12/15/2006

KOH II → I

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\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 12:29:37 ON 15 DEC 2006

=> file casreact  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 12:29:52 ON 15 DEC 2006  
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FILE CONTENT:1840 - 11 Dec 2006 VOL 145 ISS 24

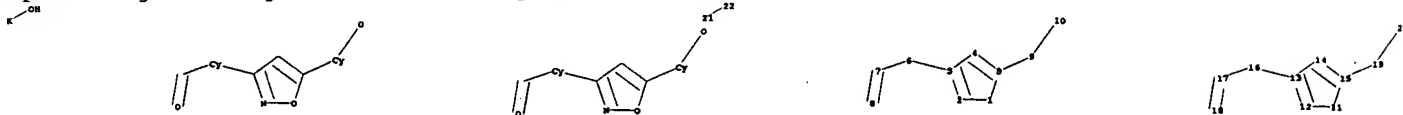
New CAS Information Use Policies, enter HELP USAGETERMS for details.

\*\*\*\*\*  
\*  
\* CASREACT now has more than 10 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Program Files\Stnexp\Queries\10522622\1.KOH+II-I.str



chain nodes :

6 7 8 9 10 16 17 18 19 20 21 22

ring nodes :

1 2 3 4 5 11 12 13 14 15

chain bonds :

3-6 5-9 6-7 7-8 9-10 13-16 15-19 16-17 17-18 19-20 21-22

ring bonds :

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1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5 5-9 6-7 7-8 9-10 11-12 11-15 12-13 13-14 13-16  
14-15 15-19 16-17 17-18 19-20

exact bonds :

21-22

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:Atom

20:CLASS 21:CLASS 22:CLASS

fragments assigned product role:

containing 11

fragments assigned reactant/reagent role:

containing 1

containing 21

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 12:30:13 FILE 'CASREACT'

SCREENING COMPLETE - 6077 REACTIONS TO VERIFY FROM 455 DOCUMENTS

100.0% DONE 6077 VERIFIED 3 HIT RXNS

2 DOCS

SEARCH TIME: 00.00.02

L2 2 SEA SSS FUL L1 ( 3 REACTIONS)

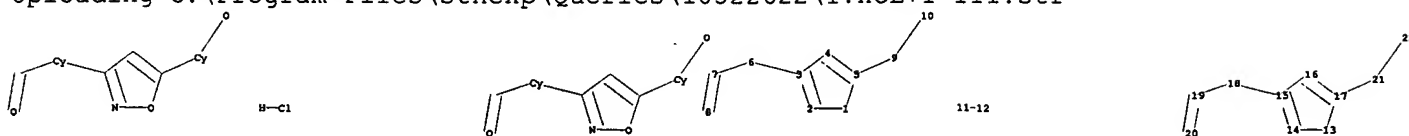
=> d ibib hit 1-2

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I nu → III

=>  
Uploading C:\Program Files\Stnexp\Queries\10522622\1.HCL+I-III.str



chain nodes :  
6 7 8 9 10 11 12 18 19 20 21 22  
ring nodes :  
1 2 3 4 5 13 14 15 16 17  
chain bonds :  
3-6 5-9 6-7 7-8 9-10 11-12 15-18 17-21 18-19 19-20 21-22  
ring bonds :  
1-2 1-5 2-3 3-4 4-5 13-14 13-17 14-15 15-16 16-17  
exact/norm bonds :  
1-2 1-5 2-3 3-4 3-6 4-5 5-9 6-7 7-8 9-10 13-14 13-17 14-15 15-16 15-18  
16-17 17-21 18-19 19-20 21-22  
exact bonds :  
11-12

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS  
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS  
20:CLASS 21:Atom 22:CLASS  
fragments assigned product role:  
containing 13  
fragments assigned reactant/reagent role:  
containing 1  
containing 11

L3 STRUCTURE UPLOADED

=> d  
L3 HAS NO ANSWERS  
L3 STR  
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

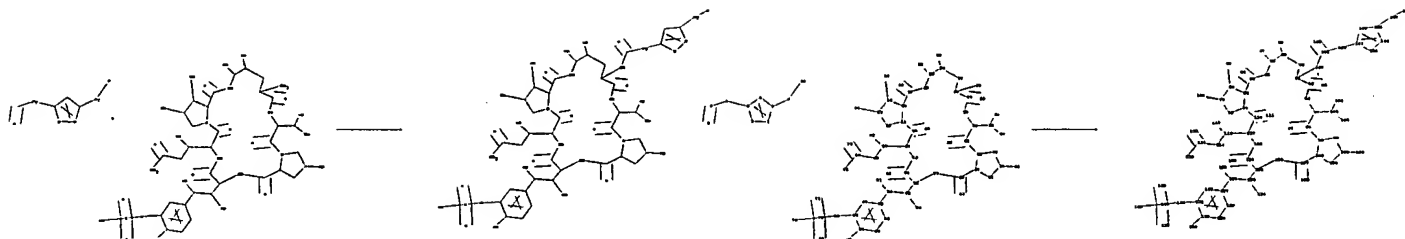
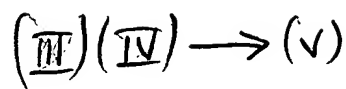
Structure attributes must be viewed using STN Express query preparation.

=> s 13 full  
FULL SEARCH INITIATED 12:31:00 FILE 'CASREACT'  
SCREENING COMPLETE - 23962 REACTIONS TO VERIFY FROM 1991 DOCUMENTS  
100.0% DONE 23962 VERIFIED 5 HIT RXNS 2 DOCS  
SEARCH TIME: 00.00.04

L4 2 SEA SSS FUL L3 ( 5 REACTIONS)

=> d ibib hit 1-2

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chain nodes :

6 7 8 9 10 16 18 21 22 26 28 32 38 39 40 41 43 44 46 48 49 50 51  
 52 55 58 59 60 61 68 69 70 71 72 73 74 82 84 87 88 93 97 103 104 105  
 106 108 109 111 113 114 115 116 117 120 123 124 125 126 133 134 135 136  
 137 138 139 140 141 142 143 149 150

ring nodes :

1 2 3 4 5 11 12 13 14 15 17 19 20 23 24 25 27 29 30 31 33 34 35 36  
 37 42 45 47 53 54 56 57 62 63 64 65 66 67 77 78 79 80 81 83 85 86  
 89 90 91 92 94 95 96 98 99 100 101 102 107 110 112 118 119 121 122 127  
 128 129 130 131 132 144 145 146 147 148

chain bonds :

3-6 5-9 6-7 7-8 9-10 13-44 14-16 17-18 20-21 22-23 25-26 27-28 30-38 31-32  
 35-41 38-39 38-40 42-43 45-46 47-48 48-49 48-52 49-50 50-51 50-73 54-55 56-58  
 58-59 58-60 60-61 60-62 65-68 66-69 69-70 70-71 70-72 70-74 79-109 80-82  
 83-84 86-87 88-89 91-140 92-93 95-103 96-97 100-106 103-104 103-105 107-108  
 110-111 112-113 113-114 113-117 114-115 115-116 115-138 119-120 121-123 123-124  
 123-125 125-126 125-127 130-133 131-134 134-135 135-136 135-137 135-139 140-141  
 141-142 141-143 143-147 145-149 149-150

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 11-45 12-13 13-14 14-15 15-17 17-19 19-20  
 20-23 23-24 24-25 25-27 27-29 29-30 30-31 31-33 33-34 33-37 34-35 35-36 36-37  
 37-42 42-57 45-47 47-53 53-54 54-56 56-57 62-63 62-67 63-64 64-65 65-66  
 66-67 77-78 77-81 77-110 78-79 79-80 80-81 81-83 83-85 85-86 86-89 89-90  
 90-91 91-92 92-94 94-95 95-96 96-98 98-99 98-102 99-100 100-101 101-102  
 102-107 107-122 110-112 112-118 118-119 119-121 121-122 127-128 127-132 128-129  
 129-130 130-131 131-132 144-148 144-145 145-146 146-147 147-148

exact/norm bonds :

1-2 1-5 2-3 3-4 3-6 4-5 5-9 6-7 7-8 9-10 11-12 11-15 11-45 12-13 13-14  
 14-15 14-16 15-17 17-18 17-19 19-20 20-21 20-23 22-23 23-24 24-25 25-26 25-27  
 27-28 27-29 29-30 30-31 31-32 31-33 33-34 33-37 34-35 35-36 35-41 36-37  
 37-42 38-39 42-43 42-57 45-46 45-47 47-53 48-52 50-51 50-73 53-54 54-55 54-56  
 56-57 58-59 60-61 65-68 66-69 69-70 77-78 77-81 77-110 78-79 79-80 80-81  
 80-82 81-83 83-84 83-85 85-86 86-87 86-89 88-89 89-90 90-91 91-92 91-140  
 92-93 92-94 94-95 95-96 96-97 96-98 98-99 98-102 99-100 100-101 100-106  
 101-102 102-107 103-104 107-108 107-122 110-111 110-112 112-118 113-117 115-116  
 115-138 118-119 119-120 119-121 121-122 123-124 125-126 130-133 131-134 134-135  
 140-141 141-142 141-143 143-147 144-148 144-145 145-146 145-149 146-147 147-148  
 149-150

exact bonds :

13-44 30-38 38-40 47-48 48-49 49-50 56-58 58-60 60-62 79-109 95-103 103-105  
 112-113 113-114 114-115 121-123 123-125 125-127

normalized bonds :

62-63 62-67 63-64 64-65 65-66 66-67 70-71 70-72 70-74 127-128 127-132 128-129  
 129-130 130-131 131-132 135-136 135-137 135-139

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:CLASS 19:Atom  
20:Atom 21:CLASS 22:CLASS 23:Atom 24:Atom 25:Atom 26:CLASS 27:Atom 28:CLASS  
29:Atom 30:Atom 31:Atom 32:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom  
38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:Atom 43:CLASS 44:CLASS 45:Atom 46:CLASS  
47:Atom 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:Atom 54:Atom 55:CLASS  
56:Atom 57:Atom 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:Atom 63:Atom 64:Atom  
65:Atom 66:Atom 67:Atom 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS  
74:CLASS 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:CLASS 83:Atom 84:CLASS  
85:Atom 86:Atom 87:CLASS 88:CLASS 89:Atom 90:Atom 91:Atom 92:Atom 93:CLASS  
94:Atom 95:Atom 96:Atom 97:CLASS 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom  
103:CLASS 104:CLASS 105:CLASS 106:CLASS 107:Atom 108:CLASS 109:CLASS 110:Atom  
111:CLASS 112:Atom 113:CLASS 114:CLASS 115:CLASS 116:CLASS 117:CLASS 118:Atom  
119:Atom 120:CLASS 121:Atom 122:Atom 123:CLASS 124:CLASS 125:CLASS 126:CLASS  
127:Atom 128:Atom 129:Atom 130:Atom 131:Atom 132:Atom 133:CLASS 134:CLASS  
135:CLASS 136:CLASS 137:CLASS 138:CLASS 139:CLASS 140:CLASS 141:CLASS 142:CLASS  
143:Atom 144:Atom 145:Atom 146:Atom 147:Atom 148:Atom 149:Atom 150:CLASS

fragments assigned product role:

containing 77

fragments assigned reactant/reagent role:

containing 1

containing 11

L5 STRUCTURE UPLOADED

=> s l5 full

FULL SEARCH INITIATED 12:46:32 FILE 'CASREACT'

SCREENING COMPLETE - 2 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 2 VERIFIED 2 HIT RXNS 1 DOCS

SEARCH TIME: 00.00.01

L6 1 SEA SSS FUL L5 ( 2 REACTIONS)

=> d ibib hit 1

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=&gt; file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

118.68

361.01

FILE 'REGISTRY' ENTERED AT 12:51:24 ON 15 DEC 2006

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Property values tagged with IC are from the ZIC/VINITI data file  
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. STRUCTURE FILE UPDATES: 14 DEC 2006 HIGHEST RN 915690-78-7

DICTIONARY FILE UPDATES: 14 DEC 2006 HIGHEST RN 915690-78-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

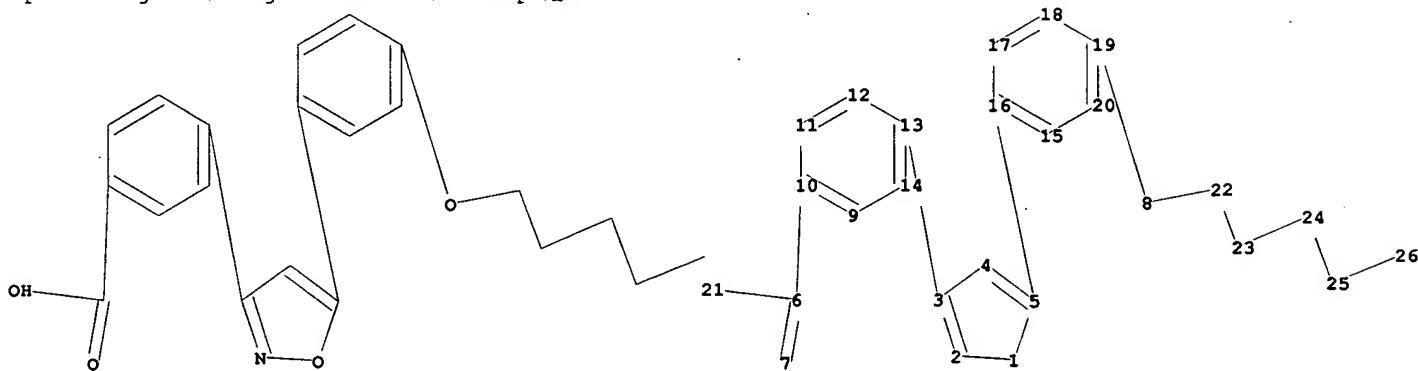
Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=&gt;

Uploading C:\Program Files\Stnexp\Queries\10522622\17.str



chain nodes :

6 7 8 21 22 23 24 25 26

ring nodes :

1 2 3 4 5 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

3-13 5-16 6-7 6-10 6-21 8-19 8-22 22-23 23-24 24-25 25-26

ring bonds :

1-2 1-5 2-3 3-4 4-5 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17

17-18 18-19 19-20

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 8-19 8-22

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exact bonds :

3-13 5-16 6-10 22-23 23-24 24-25 25-26

normalized bonds :

6-7 6-21 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17 17-18 18-19  
19-20

Match level :

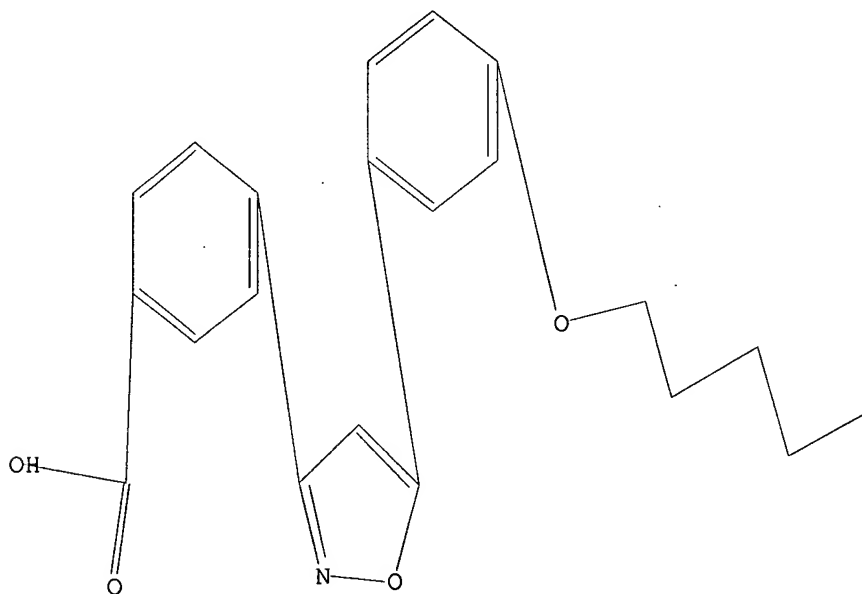
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom  
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L7 STRUCTURE UPLOADED

=> d

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17 full

FULL SEARCH INITIATED 12:51:39 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 402 TO ITERATE

100.0% PROCESSED 402 ITERATIONS

7 ANSWERS

SEARCH TIME: 00.00.01

L8 7 SEA SSS FUL L7

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

527.95

FILE 'CAPLUS' ENTERED AT 12:51:43 ON 15 DEC 2006

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FILE COVERS 1907 - 15 Dec 2006 VOL 145 ISS 26  
FILE LAST UPDATED: 14 Dec 2006 (20061214/ED)

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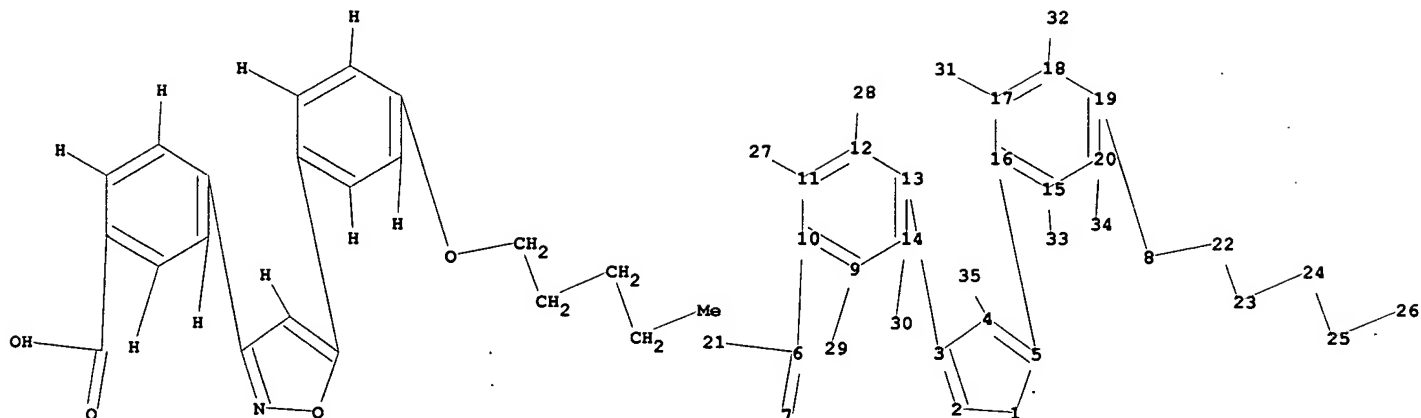
=> s 18

L9                    5 L8

=> d ibib hitstr 1-5

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```

chain nodes :
6 7 8 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35
ring nodes :
1 2 3 4 5 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
3-13 4-35 5-16 6-7 6-10 6-21 8-19 8-22 9-29 11-27 12-28 14-30 15-33 17-31
18-32 20-34 22-23 23-24 24-25 25-26
ring bonds :
1-2 1-5 2-3 3-4 4-5 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17
17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 8-19
exact bonds :
3-13 4-35 5-16 6-10 8-22 9-29 11-27 12-28 14-30 15-33 17-31 18-32 20-34
22-23 23-24 24-25 25-26
normalized bonds :
6-7 6-21 9-10 9-14 10-11 11-12 12-13 13-14 15-16 15-20 16-17 17-18 18-19
19-20

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS

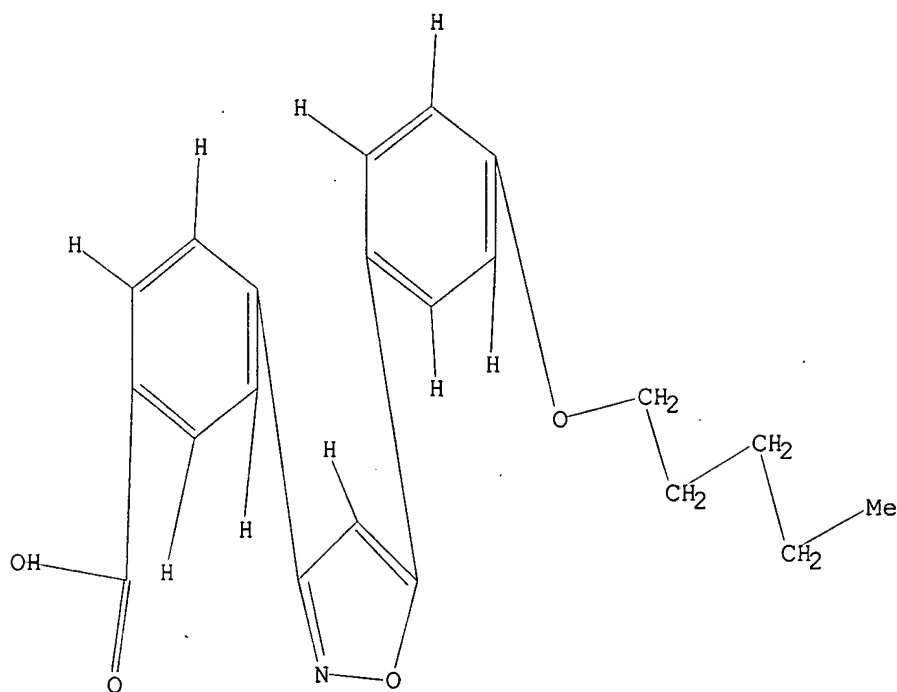
```

L1 STRUCTURE UPLOADED

```

=> d
L1 HAS NO ANSWERS
L1 STR

```



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 13:02:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 402 TO ITERATE

100.0% PROCESSED 402 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

L2 3 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'CAPLUS' ENTERED AT 13:03:03 ON 15 DEC 2006

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FILE COVERS 1907 - 15 Dec 2006 VOL 145 ISS 26  
FILE LAST UPDATED: 14 Dec 2006 (20061214/ED)

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They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 12

L3 3 L2

=> d ibib hitstr 1-3

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